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The application of the convolution relations in the X-ray line breadth studies on lattice defects

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A set of new convolution relations, from an application of simultaneous convolutions of several analytical functions representing the instrumental profile and the true diffraction profile which result from microstructural changes in materials, has been derived as a function of respective integral breadths. For the instrumental profile, favourable gaussian and double-square forms and for the true profile, an alternative representation of Schoening's (Schoening 1965) realistic cases, which arises from a convolution of double-square distribution of particle-size profile and a gaussian and a double-square strain profile, have been considered and applied to several cold-worked copper-and silver-base alloys and vapour-deposited silver films. An overall study in terms of percentage deviations in the observed integral breadths of the profiles reveals that the present alternative representation of true profile is equally applicable in the line breadth studies and pure double-square distribution function representing the instrumental as well as the true diffraction profile also approaches close to the actual case. It also turns out that the pure gaussian and pure Cauchy distributions form the two extreme cases, and all the four cases arising from Schoening's type of consideration represent an intermediate form close to the parabolic case.

1. Introduction

Extensive studies in the past on a large number of cold-worked metals and alloys (Warren 1959, 1969, Wilson 1962, Wagner 1966; Chatterjee, Halder & Sen Gupta 1976) have clearly demonstrated that the experimentally observed X-ray diffraction profile from these materials results from a convolution of the instrumental profile and the true diffraction profile, which is again a convolution of particle-size, strain and stacking fault distribution functions. Recently, we have made a series of investigations (Nandi and Sen Gupta 1975, 1976a,b; referred to as I, II and III respectively) dealing with the simultaneous convolutions of the different appropriate functional forms which may closely represent the respective profiles, and have emphasized the need for such convolutions in the line breadth studies. In these investigations we have considered both the cases (a) and (b) of Schoening's realistic representation of true diffraction profile (Schoening 1965) together with the instrumental profile having several functional forms namely, gaussian, cauchy, exponential, and double-square. From these analyses in I, II and III, applied to several cold-worked f.c.c. alloys and vapour-deposited silver films, it has turned out that both the cases (a) and (b) of Schoening's true diffraction profile (i.e. Cauchy particle-size, and gaussian and double-square strain profiles) when convoluted with the gaussian as well as double-square type instrumental profile may represent the realistic case in a fairly satisfactory manner. In the present investigation we consider, for the first time, an alternative representation of the true diffraction profile (which may be termed as case (c) and case (d) of Schoening's type of representation) resulting from a double-square particle-size profile and a gaussian and double-square strain profile and convolute these with the more favourable gaussian and double-square instrumental profile (I and II). The consideration of a double-square particle size profile in the present analysis is justifiable from its analytical form which approaches close to a gaussian case. The application has been made to same alloy and film specimens as considered in our earlier work in I-III, and an overall study has been made considering all the four cases (a), (b), (c) and (d) of true profile representation in order to see, along with the applicability of the present alternative distribution functions, the most favourable type of distribution functions for description of the X-ray diffraction profiles which originate from the materials containing imperfections.

2. Theoretical Formulations of Convolution Relations

Considering the property of Fourier transform T and its inverse the experimentally observed intensity profile $I_{obs}(x)$ can be expressed as (Nandi & Sen Gupta 1975, I)

$$I_{obs}(x) = T^{-1} < T[I_s(x)]\, T[I_p(x)].T[I_i(x)] > \qquad \dots \quad (1)$$

where $I_s(x)$, $I_p(x)$ and $I_i(x)$ represent respectively the strain profile, the particle-size profile and the instrumental pofile.

The observed integral breadth is given by

$$B_{obs}(x) = \int_{-\infty}^{\infty} I_{obs}(x)dx/I_{obs}(0) \qquad \dots \quad (2)$$

where

$$\left.\begin{aligned} \int_{-\infty}^{\infty} I_{obs}(x)dx &= < T[I_s(x)].T[I_p(x)].T[I_i(x)] >_{u=0} \\ \text{and} \quad I_{obs}(0) &= \{T^{-1} < T[I_s(x)]\, T[I_p(x)].T[I_i(x)] > \}_{x=0} \end{aligned}\right\} \qquad \dots \quad (3)$$

Here x and u are the variables in real and Fourier space respectively.

The following functions namely, gaussian and double-square with their respective Fourier transforms and integral breadths have been considerd here

(Schoening 1965, Nandi and Sen Gupta 1975, 1976a) for the purpose of simultaneous convolutions :

gaussian : $f(x) = C_g \exp(-k_g^2 x^2)$; $T[f(x)] = \pi^{\frac{1}{2}} C_g k_g^{-1} \exp(-\pi^2 u^2/k g^2)$

$$B_g = \pi^{\frac{1}{2}}/k_g \quad \ldots \quad (4)$$

double-square : $$f(x) = C_{ds}/(1+k_{ds}^2 x^2)^2 \quad \ldots \quad (5)$$

$$T[f(x)] = \tfrac{1}{2}\pi C_{ds} k_{ds}^{-2}(k_{ds}+2\pi\,|u|)\exp(-2\pi\,|u|/k_{ds}); \quad B_{ds} = \pi/2k_{ds}$$

We now formulate the two alternative cases of Schoening's true diffraction profile representation before we proceed for the simultaneous convolutions for each case considering the instrumental profile

(i) *Convolutions of double-square (particle-size) and gaussian (strain) profile : Case (c) of Schoening's representation*

The convolution of the functions leads to the following expressions for true broadth :

$$B_T \text{ (true broadth)} = B_S \exp(-H^2)[(1-erf H)(1-2H^2)+2\pi^{-\frac{1}{2}}H \exp(-H^2)]^{-1}$$

where
$$H = 2B_P/\pi^{\frac{1}{2}}B_s \quad \text{and} \quad \operatorname{erf} H = 2\pi^{-\frac{1}{2}} \int_0^H \exp(-t^2)dt \quad \ldots \quad (6)$$

with the abbreviations as before (Schoening 1965)

$$\left.\begin{aligned} B_i &= B_{iT}\cos\theta_i/\lambda \\ u_i &= Le\sin\theta_i/\lambda \\ a &= \sin\theta_1/\sin\theta_2 \end{aligned}\right\} i = 1, 2 \quad \ldots \quad (7)$$

we have

$$\frac{B_1}{B_2} = a\exp(P_1^2-P_2^2)[(1-\operatorname{erf} P_1)(1-2P_1^2)+2\pi^{-\frac{1}{2}}P_1\exp(-P_1^2)]\times$$
$$[(1-\operatorname{erf} P_2)(1-2P_2^2)+2\pi^{-\frac{1}{2}}P_2\exp(-P_2^2)]^{-1} \quad \ldots \quad (8)$$

and

$$\frac{1}{LB_2} = u_2^{-1}\exp(P_1^2)[(1-\operatorname{erf} P_1)(1-2P_1^2)+2\pi^{-\frac{1}{2}}P_1\exp(-P_1^2)]$$

where $$P_1 = 2/\pi^{\frac{1}{2}}u_2 \quad \text{and} \quad P_2 = 2/\pi^{\frac{1}{2}}au_2$$

(ia) *Convolutions of case (c) with quassian type instrumental profile*

The convolution of the functions yields for the total observed breadth :

$$B_{iG}(\text{obs}) = 2B_P D^{-1}\exp(-D^2)[\pi^{\frac{1}{2}}(1-2D^2)(1-\operatorname{erf} D)+2D\exp(-D^2)]^{-1} \quad (9)$$

where $D = 2B\nu/\pi^{\frac{1}{2}}(B_l^2+B_S^2)^{\frac{1}{2}}$; B_l, B_p, B_s denote the corresponding instrumental, particle size, and strain breadths.

(ib) *Convolutions of case (c) with double-square type instrumental profile*

The convolution of the functions in this case gives rise to :

$$B_{l-ds}(\text{obs}) = \pi \exp(-F^2)[(1-\text{erf } F)(1-2F^2+2QF^2B_s)\pi B_s^{-1}+$$
$$+2\pi^{\frac{1}{2}}F(B_s^{-1}-2Q)\exp(-F^2)+\pi Q-2\pi^{\frac{1}{2}}Q\xi(3/2, F^2)]^{-1} \quad \ldots \quad (10)$$

where

$$F = 2(B_l+B_p)/\pi^{\frac{1}{2}}B_s; \quad Q = 8B_lB_p/\pi B_s^3$$

and

$$\xi(3/2, F^2) = \int_0^{F^2} t^{\frac{1}{2}} \exp(-t)dt$$

(ii) *Convolution of double-square (particle-size) and double-square (strain profile): case (d) of Schoening's representation*

In this case the true breadth is given by

$$B_T = (B_s+B_p)\left[1+\frac{B_sB_p}{(B_s+B_p)^2}\right]^{-1} \quad \ldots \quad (11)$$

with the same abbreviations (7), we have

$$\left.\begin{aligned} \frac{B_1}{B_2} &= \left(\frac{au_2+1}{u_2+1}\right)^3 \frac{u_2^2+3u_2+1}{a^2u_2^2+3au_2+1} \\ &\text{and} \\ \frac{1}{LB_2} &= \frac{u_2^2+3u_2+1}{(u_2+1)^3} \end{aligned}\right\} \quad \ldots \quad (12)$$

(iia) *Convolutions of case (d) with gaussian type instrumental profile*

The convolution of the functions gives for the observed breadth :

$$B_{lG}(\text{obs}) = \pi \exp(-P^2)[(1-\text{erf } P)(1-2P^2+2B_lRP^2)\pi B_l^{-1}+$$
$$2\pi^{\frac{1}{2}}P(B_l^{-1}-2R)\exp(-P^2)+\pi R-2\pi^{\frac{1}{2}}R\xi(3/2, P^2)]^{-1} \quad \ldots \quad (13)$$

where $\quad P = 2(B_s+B_p)/\pi^{\frac{1}{2}}B_l \quad$ and $\quad R = 8B_sB_p/\pi B_l^3$

(iib) *Convolutions of case (d) with double-square type instrumental profile*

In this case of representation, we have for the observed breadth

$$B_{l-ds}(\text{obs}) = \frac{\pi A}{2}\left[1+\frac{1}{A^2B}\left(C+\frac{3}{A}\right)\right]^{-1} \quad \ldots \quad (14)$$

where

$$A = \frac{2}{\pi}(B_l+B_p+B_s); \quad B = \frac{\pi^3}{8}\,\frac{1}{B_lB_sB_p}$$

and

$$C = \frac{\pi}{2} \frac{B_l B_p + B_l B_s + B_s B_p}{B_l B_p B_s}$$

The integral breadths B_s and B_p are related to the parameters namely strain (e) and particle size (L) by the following relations,

$$B_s = e \tan\theta \quad \text{and} \quad B_p = \lambda/L \cos\theta \qquad \ldots \quad (15)$$

3. Results and Discussion

Tables 1a and 1b show the respective values for particle-size $L(\text{Å})$ and strain ϵ determined from all the four cases (a), (b), (c) and (d) of Schoening's representation considering an intermediate parabolic type of instrumental broadening correction along with those from pure gaussian and pure Cauchy cases for silver— and copper base alloys and vapour-deposited silver films (Nandi & Sen Gupta 1975, 1976a, Chatterjee & Sen Gupta 1972; Sen *et al* 1975). In table 2, the experimental B_{expt}(obs) values and those calculated from cases (ia), (ib), (iia) and (iib) representing Schoening's case (c) and case (d) along with percentage deviations observed for all the four cases of representation have been tabulated for an overall comparison. The numerical calculations have been done on an IBM 1130 computer utilizing suitable programs.

From tables 1a & 1b it now appears that there exists a fairly satisfactory agreement in the values for the effective particle size and micro-strain for all the four cases (a), (b), (c) and (d) as the respective values are considerably closer. It may be seen (Table 1a) that the particle-size values $L(\text{Å})$ are not much influenced as we go from Cauchy to double-square type of distributions for the particle-size profile and there exists a very good agreement for the two cases (b) and (d). As regards strain values ϵ (Table 1b), the assumption on particle size distribution functions has, however, a little influence since the values for cases (a) and (b) which are quite close to each other deviate slightly from those for cases (c) and (d). However, for a particular type of distribution function representing the particle-size profile, the gaussian or double-square distribution function hardly results in an appreciable difference in the strain values, as may be evident from cases (a), (b) and cases (c), (d). The pure gaussian and Cauchy cases have always been found to yield the two extreme cases for the particle-size D ($= L(\text{Å})$) and strain ϵ ($= 4e$) and these deviate considerably from the Schoening's realistic representations which are in fact close to the parabolic representation (Chatterjee and Sen Gupta 1972) and thereby appear as intermediate cases.

In table 2, where the percentage deviations in B (obs) have been estimated from the calculated and experimental values, it turns out that the Schoening's alternative representations (cases (c) and (d)) of double-square type of particle-

Table 1a : Particle size values L, D (Å) obtained from different cases of of Schoening's representation and also from pure gaussian and Cauchy cases for the silver-and copper-base alloys and silver films

Composition	Case (a)		Case (b)		Case (c)		Case (d)		Pure Gaussian*		Pure Cauchy*	
	L_{111}	L_{100}	L_{111}	L_{100}	L_{111}	L_{100}	L_{111}	L_{100}	D_{111}	D_{100}	D_{111}	D_{100}
Cu-1.05% Sb	208	180	223	173	214	154	226	169	200	140	278	227
Cu-3.23% Sb	216	178	213	164	189	130	208	149	177	117	270	219
Cu 5.79% Sb	149	90	113	83	129	72	142	81	122	67	185	111
Ag-22.54% Zn	245		253		222		245		202		344	
Ag-32.94% Zn	205		211		192		209		182		278	
Ag-2.66% Sb	198	111	207	107	198	98	210	107	180	92	256	141
Ag-4.00% Sb	194	96	190	91	176	83	192	90	160	78	244	120
Ag film ~1113 Å	337		318		309		323		296		394	
Ag film 1291Å	356		331		306		332		295		420	
Ag film ~1691Å	345		322		305		326		292		400	
Ag film ~1853Å	461		442		428		446		426		513	
Ag film ~2125Å	456		428		405		430		392		526	

*Chatterjee and Sen Gupta (1972)
*Sen et al (1975)

size distribution when convoluted with the more favourable gaussian or double-square type of instrumental profile (II, Nandi and Sen Gupta 1976a) also approach very close to the realistic case (b), as the deviations in most of the results lie within 1%, which has also been observed earlier in I and II. In the case of silver films the deviation is slightly enhanced for the case (c) convoluted with gaussian instrumental profile only. However, the functional form (eqn. (13)) for case (d) which resulted from convoluion with gaussian instrumental profile does not permit us to calculate B(obs) in case of highly deformed alloy specimens and thin silver films. Similar limitation also arose earlier in II (Nandi and Sen Gupta 1976a) with case (a) convoluted with the gaussian instrumental profile

From an overall analysis on the application of the convolution relations derived here and also earlier in I and II to X-ray line breadth studies on materials containing appreciable lattice imperfections, we may derive the following important conclusions

Table 1b. Strain values ϵ, ϵ (10^{-3}) obtained from different cases of Schoening's representation and also from pure Gaussian and Cauchy cases for the silver- and-copper-base alloys and silver films

Composition	Case (a) 111	Case (a) $_{\epsilon}100$	Case (b) $_{\epsilon}111$	Case (b) $_{\epsilon}100$	Case (c) $_{\epsilon}111$	Case (c) $_{\epsilon}100$	Case (d) $_{\epsilon}111$	Case (d) $_{\epsilon}100$	Pure Gaussian* $\epsilon^{c}111$	Pure Gaussian* $\epsilon^{c}100$	Pure Cauchy* $\epsilon^{c}111$	Pure Cauchy* $\epsilon^{c}100$
Cu-1.05% Sb	8.78	17.55	9.77	18.25	11.73	21.11	11.09	20.45	3.19	5.54	2.16	4.36
Cu-3.23% Sb	17.54	36.87	18.22	37.01	20.91	40.59	20.44	39.83	5.48	10.36	4.37	9.12
Cu-5.79% Sb	23.73	45.22	24.29	46.57	28.75	52.84	27.87	51.21	7.55	13.71	5.89	11.25
Ag-22.54% Zn	17.64		18.47		21.41		20.44		5.48		4.43	
Ag-32.94% Zn	16.63		17.62		20.55		19.95		5.41		4.19	
Ag-2.66% Sb	11.37	28.68	12.02	29.65	14.99	34.50	14.20	33.15	4.03	9.12	2.77	6.98
Ag-4.00% Sb	17.15	33.41	17.50	35.94	21.00	40.88	20.27	39.63	5.54	10.84	4.15	8.32
Ag film ~1113Å	7.54		7.77		9.33		8.93		2.57		1.76	
Ag film ~1291Å	9.77		9.96		11.81		11.35		3.14		2.35	
Ag film ~1691Å	8.18		8.40		10.23		9.72		2.76		1.96	
Ag film ~1853Å	4.08		4.26		5.33		4.94		1.49		0.92	
Ag film ~2125Å	5.93		6.05		7.34		6.94		1.99		1.39	

* Chatterjee and Sen Gupta (1972) ; *Sen et al (1975)

Table 2. Experimental and calculated B(obs) with their percentage deviations for the copper- and silver-base alloys and silver films considering cases (a), (b) (Nandi and Sen Gupta 1975, 1976a) and cases (c), (d) of Schoening's representation

Composition	hkl	B (obs) (expt.) (deg)	B_{IG} (obs) (calc.) (deg) Case (c)	B_{IG} (obs) (calc.) (deg) Case (d)	% deviation of B_{IG}(obs) Case (a) : II	Case (b) : I	Case (c)	Case (d)
Cu-1.05 a/o Sb	111	0.5802	0.5679			−0.16	+2.11	
	222	1.0456	1.0335			−0.13	+1.18	
	200	0.9168	0.9150			−0.79	+0.19	
	400	2.3750	2.3734			−0.01	+0.07	
Cu-3.23 a/o Sb	111	0.7520	0.7463			+0.18	+0.76	
	222	1.5522	1.5471			−1.06	+0.32	
	200	1.4152	1.4118			+0.18	+0.23	
	400	4.0400	4.0310			−1.10	+0.22	
Cu-5.79 a/o Sb	111	1.0498	1.0495			−0.05	+0.02	
	222	2.1282	2.1329			−1.84	−0.22	
	200	2.0698	2.0779			−0.28	−0.39	
	400	5.4133	5.4308			+0.70	−0.32	
Ag-22.54 a/o Zn	111	0.6610	0.6571			−0.43	+0.58	
	222	1.2630	1.2731			−0.10	−0.82	
Ag-32.94 a/o Zn	111	0.7050	0.6973			+0.28	+1.10	
	222	1.2960	1.2968			−0.08	+0.24	
Ag-2.66 a/o Sb	111	0.6164	0.6067			−0.32	+1.58	
	222	1.0240	1.0169			−1.22	+0.68	
	200	1.3600	1.3547			−0.79	+0.39	
	400	2.8070	2.8031			−0.26	+0.14	
Ag-4.00 a/o Sb	111	0.7286	0.7242			−1.88	+0.61	
	222	1.3068	1.3033			−1.17	+0.27	
	200	1.5911	1.5894			+1.23	+0.11	
	400	3.2901	3.2923			+0.93	−0.07	
Ag film ~1113 Å	111	0.4647	0.4342		+1.33	−0.58	+6.55	
	222	0.6846	0.7039			+6.77	−2.82	
~1291 Å	111	0.4893	0.4634		−0.31	−2.18	+5.29	
	222	0.8365	0.7991		−0.64	−2.90	+4.47	
~1691 Å	111	0.4721	0.4466		+0.53	+0.23	+5.41	
	222	0.7792	0.7398		−0.83	−2.29	+5.05	
~1851 Å	111	0.3633	0.3363	0.3409	+2.01	+1.14	+7.42	+6.18
	222	0.5512	0.5050	0.5401	+0.03	−2.64	+8.38	+2.01
~2125 Å	111	0.3896	0.3619	0.3801	+0.97	+0.56	+7.12	+2.43
	222	0.6228	0.5777		−0.46	−3.88	+7.24	

Composition	hkl	B_{t-ds} (obs) (expt.) (deg)	B_{t-ds} (obs) (calc.) (deg) Case (c)	B_{t-ds} (obs) (calc.) (deg) Case (d)	% deviation of B_{t-ds} (obs) Case (a) : II	Case (b) : II	Case (c)	Case (d)
Cu-1.05 a/o Sb	111	0.5802		0.5886	+10.98	+4.27		−1.46
	222	1.0456	1.0522	1.0563	+5.58	+2.14	−0.41	−0.99
	200	0.9168	0.9251	0.9227	+2.07	+0.57	−0.90	−0.65
	400	2.3750	2.3860	2.3802	+0.36	+0.05	−0.46	−0.22
Cu-3.23 a/o Sb	111	0.7520	0.7586	0.7606	+4.37	+1.28	−0.88	−1.14
	222	1.5522	1.5572	1.5624	+1.14	+0.22	0.33	−0.66
	200	1.4152	1.4238	1.4126	+2.04	+0.39	−0.61	−0.07
	400	4.0400	4.0580	4.0375	+1.43	+0.19	−0.43	+0.06
Cu-5.79 a/o Sb	111	1.0498	1.0604	1.0556	+2.29	0.19	−1.02	−0.56
	222	2.1282	2.1395	2.1316	+0.20	−1.10	−0.53	−0.16
	200	2.0698	2.0829	2.0552	+0.42	+0.68	−0.64	+0.70
	400	5.1133	5.4354	5.3672	−2.59	+0.09	−0.41	+0.85
Ag-22.54 a/o Zn	111	0.6610	0.6719	0.6690	+6.94	+1.91	−1.66	−1.21
	222	1.2630	1.2850	1.2687	+2.74	+0.67	−1.74	−0.46
Ag-32.94 a/o Zn	111	0.7050	0.7147	0.7151	+6.65	+2.06	−1.37	−1.44
	222	1.2960	1.3030	1.3072	+2.31	+0.52	0.54	−0.87
Ag-2.66 a/o Sb	111	0.6164		0.6252	+9.37	+3.00		−1.43
	222	1.0240	1.0291	1.0316	+4.38	0.09	−0.53	−0.84
	200	1.3600	1.3732	1.3702	+3.84	+1.57	−0.97	−0.75
	400	2.8070	2.8168	2.8180	+1.82	+0.64	−0.35	−0.39
Ag-4.00 a/o Sb	111	0.7286	0.7385	0.7331	+4.77	+1.07	−1.36	−0.61
	222	1.3968	1.3119	1.3109	+2.19	−0.63	−0.39	−0.32
	200	1.5911	1.6005	1.6023	−0.99	+1.68	−0.59	−0.71
	400	3.2901	3.2981	3.3010	−0.53	+1.78	−0.24	−0.33
Ag film ~1113 Å	111	0.4647		0.4669	+6.95	+5.85		−0.47
	222	0.6846						
~1291 Å	111	0.4893		0.4921	+5.76	+4.17		−0.58
	222	0.8365	0.8336	0.8456	+4.04	+1.53	+0.35	−1.09
~1691 Å	111	0.4721		0.4747	+6.08	+5.13		−0.56
	222	0.7792	0.7755	0.7863	+4.12	+1.82	+0.47	−0.91
~1853 Å	111	0.3633		0.3599	+7.78		–	+0.91
	222	0.5512		0.5478	+5.88	+3.47		+0.62
~2125 Å	111	0.3896		0.3882	+6.80			+0.36
	222	0.6228	0.6173	0.6246	+5.20	+2.20	+0.38	−0.28

(1) The proposed alternative representation of true diffraction profile does not deviate significantly from the original representations of Schoening (1965). This, therefore, envisages a Cauchy as well as double-square distributions for particle-size along with the gaussian and double-square distributions for microstrains.

(2) The instrumental profile and the strain profile may as well be represented by a double-square distribution as well as a gaussian one.

(3) A pure double-square distribution function for the instrumental, particle-size, and strain profile also approaches close to the actual case, and may, therefore be considered to be a favourable distribution function for representing the X-ray line broadening effects

(4) Pure gaussian and pure Cauchy distribution functions are the two extreme cases, and all the cases (a), (b) (c) and (d), arising from Schoening's consideration (Schoening 1965), represent an intermediate form close to the simpler parabolic case of Halder the Wagner (1966)

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